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STRUCTURE FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8  
 DICTIONARY FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

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TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

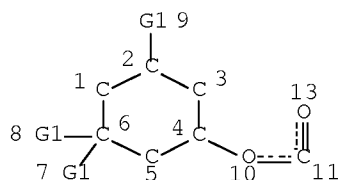
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 on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=> d sta que l14

L12 STR



VAR G1=AK/ID

NODE ATTRIBUTES:

CONNECT IS M1 RC AT 11

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 4

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L14 432 SEA FILE=REGISTRY CSS FUL L12

100.0% PROCESSED 527973 ITERATIONS

432 ANSWERS

SEARCH TIME: 00.00.07

=> fil hcplus

FILE 'HCPLUS' ENTERED AT 09:58:28 ON 27 OCT 2008  
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FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18  
 FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d 137 bib abs hitstr retable tot

L37 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN

AN 2005:96462 HCAPLUS Full-text

DN 142:161998

TI Cis-3,3,5-trimethylcyclohexyl esters for use as fragrances

IN Kuhn, Walter; Surburg, Horst

PA Symrise GmbH & Co. Kg, Germany

SO PCT Int. Appl., 33 pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005009492	A1	20050203	WO 2004-EP51292	20040630 <--
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	DE 10332908	A1	20050210	DE 2003-10332908	20030719 <--
	EP 1648526	A1	20060426	EP 2004-741922	20040630 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
	US 20060211597	A1	20060921	US 2006-565241	20060119 <--
PRAI	DE 2003-10332908	A	20030719 <--		
	WO 2004-EP51292	W	20040630 <--		
OS	MARPAT 142:161998				

AB The invention relates to mixts. of cis-3,3,5-trimethylcyclohexyl esters with trans-3,3,5-trimethylcyclohexyl esters, the use of cis-3,3,5-trimethylcyclohexyl esters as fragrances and individual cis-3,3,5-trimethylcyclohexyl esters and their use as fragrances. Thus 3,3,5-trimethylcyclohexyl acetate was synthesized from 3,3,5-trimethylcyclohexanol and acetic acid anhydride; the product contained 90% cis-3,3,5-trimethylcyclohexyl acetate. It was used in a fragrance composition as 65 weight part ingredient; other components were (weight parts): benzyl acetate 30; Ozonil (2-Tridecennitrile) 10% in diethylphthalate 5; dihydromyrcenol 150; decanal 1; 2-phenoxyethylisobutyrate 100; methylcedrylketon 35; hexyl cinnamic aldehyde 50; Lilial 30; linalyl acetate 100; Galaxolide 50% in diethylphthalate 10; cedryl acetate 30; Zibeth absolute synth. 1; lemon terpene 70; ethylvanillin 3;  $\gamma$ -undecalactone 1; citronitril 10; Projasmon P (2-heptylcycloheptanon) 1; Agrumex HC (2-tert.-butylcyclohexyl acetate) 30; hexenyl isobutyrate, cis/trans- 1; hexenylacetate cis/trans- 1; Limette oil, synth. 10; diethylphthalate 2.66.

IT 828912-43-2P 828912-45-4P 828912-47-6P

RL: COS (Cosmetic use); PRP (Properties); SPN (Synthetic preparation);

BIOL (Biological study); PREP (Preparation); USES (Uses)

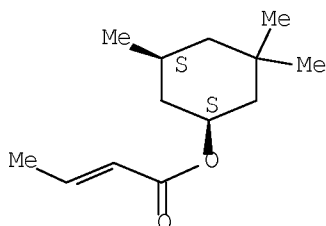
(cis-3,3,5-trimethylcyclohexyl esters for use as fragrances)

RN 828912-43-2 HCAPLUS

CN 2-Butenoic acid, (1R,5R)-3,3,5-trimethylcyclohexyl ester, rel- (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry unknown.

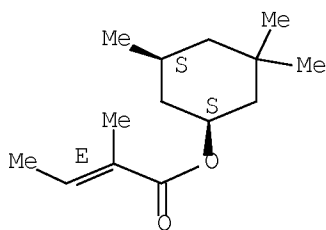


RN 828912-45-4 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1R,5R)-3,3,5-trimethylcyclohexyl ester, (2E)-rel- (CA INDEX NAME)

Relative stereochemistry.

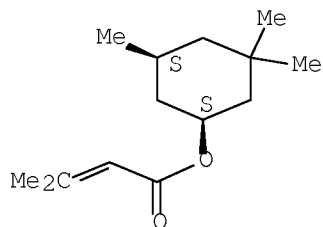
Double bond geometry as shown.



RN 828912-47-6 HCAPLUS

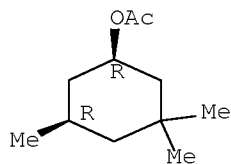
CN 2-Butenoic acid, 3-methyl-, (1R,5R)-3,3,5-trimethylcyclohexyl ester, rel- (CA INDEX NAME)

Relative stereochemistry.



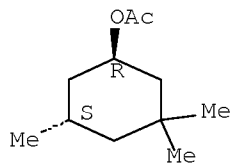
IT 24691-16-5P 24691-18-7P 60234-70-0P  
 60234-71-1P 828912-37-4P 828912-38-5P  
 828912-39-6P 828912-40-9P 828912-41-0P  
 828912-42-1P 828912-44-3P 828912-46-5P  
 828912-48-7P  
 RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (cis-3,3,5-trimethylcyclohexyl esters for use as fragrances)  
 RN 24691-16-5 HCAPLUS  
 CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate, (1R,5R)-rel- (CA INDEX NAME)

Relative stereochemistry.



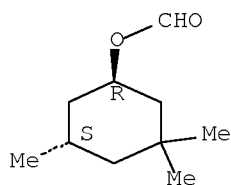
RN 24691-18-7 HCAPLUS  
 CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate, (1R,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 60234-70-0 HCAPLUS  
 CN Cyclohexanol, 3,3,5-trimethyl-, formate, (1R,5S)-rel- (9CI) (CA INDEX NAME)

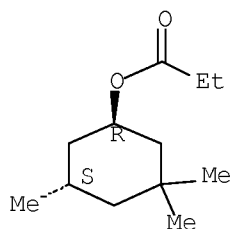
Relative stereochemistry.



RN 60234-71-1 HCAPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, propanoate, (1R,5S)-rel- (9CI) (CA INDEX NAME)

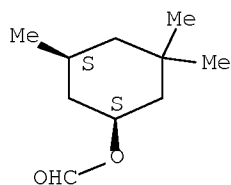
Relative stereochemistry.



RN 828912-37-4 HCAPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, 1-formate, (1R,5R)-rel- (CA INDEX NAME)

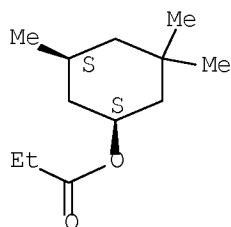
Relative stereochemistry.



RN 828912-38-5 HCAPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, 1-propanoate, (1R,5R)-rel- (CA INDEX NAME)

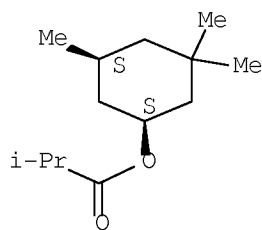
Relative stereochemistry.



RN 828912-39-6 HCAPLUS

CN Propanoic acid, 2-methyl-, (1R,5R)-3,3,5-trimethylcyclohexyl ester, rel-  
(CA INDEX NAME)

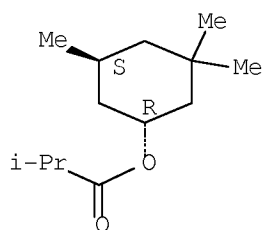
Relative stereochemistry.



RN 828912-40-9 HCAPLUS

CN Propanoic acid, 2-methyl-, (1R,5S)-3,3,5-trimethylcyclohexyl ester, rel-  
(CA INDEX NAME)

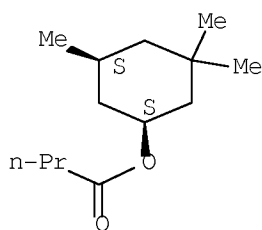
Relative stereochemistry.



RN 828912-41-0 HCAPLUS

CN Butanoic acid, (1R,5R)-3,3,5-trimethylcyclohexyl ester, rel- (CA INDEX  
NAME)

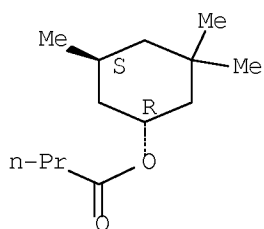
Relative stereochemistry.



RN 828912-42-1 HCAPLUS

CN Butanoic acid, (1R,5S)-3,3,5-trimethylcyclohexyl ester, rel- (CA INDEX  
NAME)

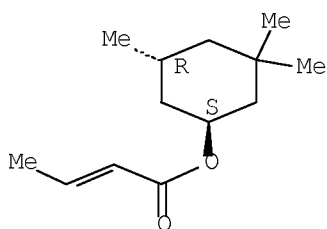
Relative stereochemistry.



RN 828912-44-3 HCAPLUS

CN 2-Butenoic acid, (1R,5S)-3,3,5-trimethylcyclohexyl ester, rel- (CA INDEX NAME)

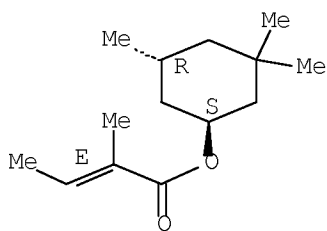
Relative stereochemistry.  
Double bond geometry unknown.



RN 828912-46-5 HCAPLUS

CN 2-Butenoic acid, 2-methyl-, (1R,5S)-3,3,5-trimethylcyclohexyl ester, (2E)-rel- (CA INDEX NAME)

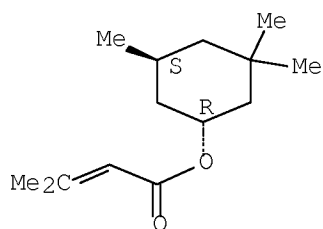
Relative stereochemistry.  
Double bond geometry as shown.



RN 828912-48-7 HCAPLUS

CN 2-Butenoic acid, 3-methyl-, (1R,5S)-3,3,5-trimethylcyclohexyl ester, rel- (CA INDEX NAME)

Relative stereochemistry.



## RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Henkel & Cie Gmbh	1976			DE 2518392 A	HCAPLUS
Merckle Kg Chem Pharm L	1974			DE 2326061 A	HCAPLUS
Poli Ind Chimica Spa	1974			DE 2406849 A	HCAPLUS
Rohde, U	2001			WO 0143784 A	HCAPLUS
Roussel-Uclaf	1970			DE 2026409 A	HCAPLUS

L37 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN

AN 2002:423916 HCAPLUS Full-text

DN 137:6868

TI High-heat resistance low-hygroscopicity (meth)acrylic resins

IN Asada, Takeshi; Kakumoto, Satoru; Takahashi, Ikuo

PA Daicel Chemical Industries, Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2002161112	A	20020604	JP 2000-361974	20001128 <--
PRAI	JP 2000-361974		20001128	<--	

AB Resins contain >3% trimethylcyclohexyl (meth)acrylate, which contains >50 mol% trans- or cis-isomer. Thus, trans-3,3,5-trimethylcyclohexyl methacrylate was prepared and polymerized with AIBN to prepare a polymer.

IT ~~433334-69-1P~~ ~~433334-70-4F~~

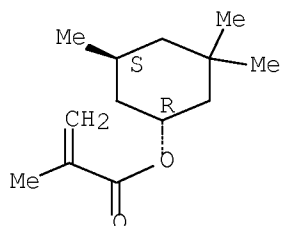
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(trimethylcyclohexyl (meth)acrylate resins)

RN 433334-69-1 HCAPLUS

CN 2-Propenoic acid, 2-methyl-, (1R,5S)-3,3,5-trimethylcyclohexyl ester, rel- (CA INDEX NAME)

Relative stereochemistry.

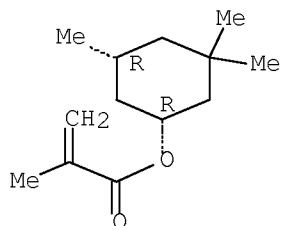




RN 433334-70-4 HCAPLUS

CN 2-Propenoic acid, 2-methyl-, (1R,5R)-3,3,5-trimethylcyclohexyl ester, rel-  
(CA INDEX NAME)

Relative stereochemistry.



L37 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN

AN 2001:452890 HCAPLUS Full-text

DN 135:66066

TI Ester odor neutralizers

IN Rohde, Ute; Hillers, Stephan; Surburg, Horst; Sonnenberg,  
Steffen; McDermott, Keith; Smith, Leslie; Sparkuhle, KarlPA Haarmann & Reimer G.m.b.H., Germany; Haarmann und Reimer  
G.m.b.H.

SO PCT Int. Appl., 52 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001043784	A2	20010621	WO 2000-EP12374	20001208
	WO 2001043784	A3	20011115		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1239890	A2	20020918	EP 2000-991148	20001208
	EP 1239890	B1	20041110		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2003516813	T	20030520	JP 2001-544920	20001208
	AT 281847	T	20041115	AT 2000-991148	20001208
	ES 2231305	T3	20050516	ES 2000-991148	20001208
	US 20030068295	A1	20030410	US 2002-149564	20020909
	US 7157411	B2	20070102		
PRAI	US 1999-170424P	P	19991213		
	WO 2000-EP12374	W	20001208		

OS MARPAT 135:66066

AB This invention relates to odor neutralizers comprising esters such as 2,4-dimethyl-3-pentyl esters of propionic, isobutyric, crotonic, and butyric

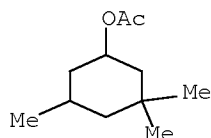
acids. These esters and a number of other similar esters were prepared and tested for their deodorant properties against sweat, ammonia, tobacco smoke, etc.

IT 67859-96-5F 94021-79-1P 94200-12-1F  
105937-88-0P 123232-56-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(ester odor neutralizers)

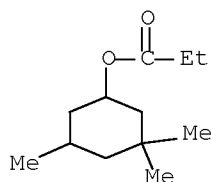
RN 67859-96-5 HCAPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)



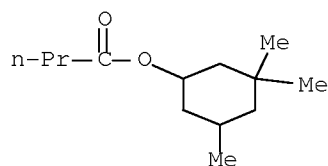
RN 94021-79-1 HCAPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, 1-propanoate (CA INDEX NAME)



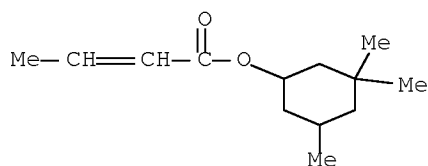
RN 94200-12-1 HCAPLUS

CN Butanoic acid, 3,3,5-trimethylcyclohexyl ester (CA INDEX NAME)

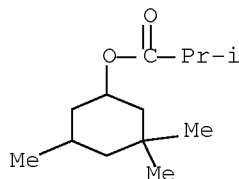


RN 105937-88-0 HCAPLUS

CN 2-Butenoic acid, 3,3,5-trimethylcyclohexyl ester (CA INDEX NAME)



RN 123232-56-4 HCAPLUS  
 CN Propanoic acid, 2-methyl-, 3,3,5-trimethylcyclohexyl ester (CA INDEX NAME)

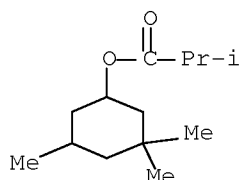


L37 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN  
 AN 1989:576823 HCAPLUS Full-text  
 DN 111:176823  
 OREF 111:29439a,29442a  
 TI Liquid detergent-bleach compositions containing perfume  
 IN Kishida, Koichi; Imanishi, Yoshitake  
 PA Taiyo Perfumery Co., Ltd., Japan  
 SO Jpn. Kokai Tokkyo Koho, 6 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 01056798	A	19890303	JP 1987-213059	19870828 <--
PRAI	JP 1987-213059		19870828	<--	

AB The compns., showing good odor-masking effects in the detergents and on laundered towels, contain hypochlorite 1-8 (as active Cl), alkali hydroxide 0.5-5, surfactant 0.1-5, and  $\geq 1$  of a list of selected perfumes 0.01-1%. A typical composition comprising NaOCl 6 (as active Cl), polyethylene glycol nonylphenyl ether sulfate Na salt 4, NaOH 3, campholenyl alc. 0.1, and water to 100% showed good odor masking, even after being stored 21 days at 45° in a polyethylene bottle.

IT 123232-56-4  
 RL: TEM (Technical or engineered material use); USES (Uses)  
 (perfumes, liquid laundry detergent-hypochlorite bleach compns. containing)  
 RN 123232-56-4 HCAPLUS  
 CN Propanoic acid, 2-methyl-, 3,3,5-trimethylcyclohexyl ester (CA INDEX NAME)



L37 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN

AN 1986:33872 HCAPLUS Full-text

DN 104:33872

OREF 104:5553a,5556a

TI Ultraviolet absorbing compounds and compositions containing these compounds

IN Baker, James Albert

PA Graesser Laboratories Ltd., UK

SO Eur. Pat. Appl., 25 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 153089	A1	19850828	EP 1985-300800	19850206 <--
	R: AT, BE, CH, DE, FR, IT, LI, LU, NL, SE				
	GB 2155467	A	19850925	GB 1985-3039	19850206 <--
	GB 2155467	B	19870325		
	US 4592906	A	19860603	US 1985-699955	19850208 <--
	AU 8538675	A	19850822	AU 1985-38675	19850213 <--
	ZA 8501081	A	19861029	ZA 1985-1081	19850213 <--
	JP 60231637	A	19851118	JP 1985-27539	19850214 <--
PRAI	GB 1984-3836	A	19840214	<--	

OS MARPAT 104:33872

AB 4-Me<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CH:CHCO<sub>2</sub>R (I; R = 2-ethylhexyl, 2-octyl) were prepared for use as UV (type A) absorbers in sunscreen compns. Thus, 40 g I (R = Et), 60 mL 2-ethylhexanol, 60 mL PhMe, and 0.1 g Na were stirred at 130° to give, after workup and vacuum distillation, 38 g I (R = 2-ethylhexyl; II). II has a m.p. of -5°, is completely miscible with both mineral oil and MeOH, and has an absorptivity of 101 at λ<sub>max</sub> = 363 nm. Several sun-block formulations were given.

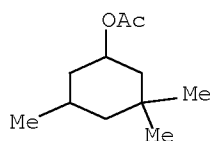
IT 67859-96-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(condensation of, with dimethylaminobenzaldehyde)

RN 67859-96-5 HCAPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate (CA INDEX NAME)



L37 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN

AN 1976:494493 HCAPLUS Full-text

DN 85:94493

OREF 85:15145a,15148a

TI Synthesis of scented compounds from isophorone

AU Podlejski, Jerzy; Wilczynska, Janina

CS Inst. Fundam. Food Chem., Lodz Polytech Univ., Lodz, Pol.

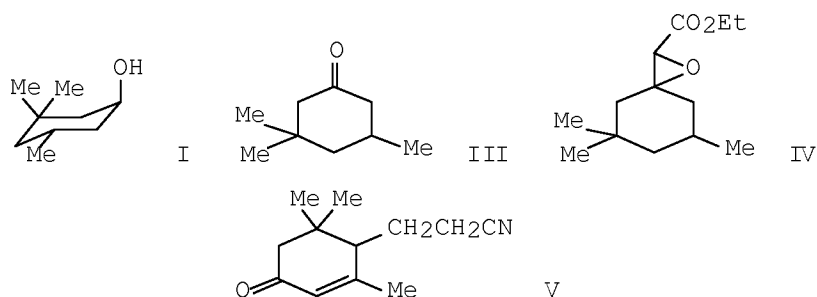
SO Tluszcze, Srodki Piorace, Kosmetyki (1975), 19(12), 516-20

CODEN: TSPKBZ; ISSN: 0372-1795

DT Journal

LA Polish

GI



AB Trans-3,3,5-Trimethylcyclohexanol (I) was obtained in 90% yield from isophorone (II) by reduction with Raney Ni 15 hr at 95° and 40 atmospheric whereas II was reduced on Ni(HCO<sub>2</sub>)<sub>2</sub> at 60° to give 98% III. Dihydroisophorone condensed with ClCH<sub>2</sub>CO<sub>2</sub>Et in PhMe containing Na at 0° gave 65% IV which was hydrolyzed and decarboxylated to give 50% 1-formyl-3,3,5-trimethylcyclohexane. Condensation of II with MeCO<sub>2</sub>CMe:CH<sub>2</sub> followed by treatment with CH<sub>2</sub>:CHCN and hydrolysis gave 60% V useful as a scent for tobacco.

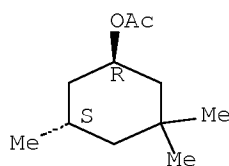
IT 24691-18-7P 60234-70-0P 60234-71-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 24691-18-7 HCAPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate, (1R,5S)-rel- (CA INDEX NAME)

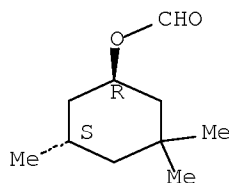
Relative stereochemistry.



RN 60234-70-0 HCAPLUS

CN Cyclohexanol, 3,3,5-trimethyl-, formate, (1R,5S)-rel- (9CI) (CA INDEX NAME)

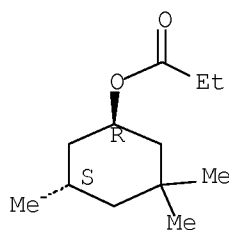
Relative stereochemistry.



RN 60234-71-1 HCAPLUS

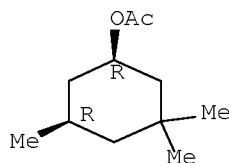
CN Cyclohexanol, 3,3,5-trimethyl-, propanoate, (1R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



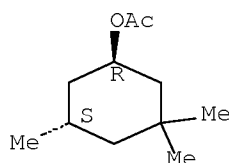
L37 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN  
 AN 1970:465956 HCAPLUS Full-text  
 DN 73:65956  
 OREF 73:10799a,10802a  
 TI Reductions with metal-ammonia combinations. II. Monothioacetals and monothioketals. Synthesis of alkoxymercaptans  
 AU Eliel, Ernest L.; Doyle, Terrence W.  
 CS Dep. of Chem., Univ. of Notre Dame, Notre Dame, IN, USA  
 SO Journal of Organic Chemistry (1970), 35(8), 2716-22  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DT Journal  
 LA English  
 OS CASREACT 73:65956  
 AB The reduction of oxathiolanes and oxathianes with metal-liquid NH<sub>3</sub> combinations gives rise to  $\beta$ - and  $\gamma$ -alkoxymercaptans. Twenty-six cases were studied; yields are good for all oxathianes and most oxathiolanes (except those with very simple 2-alkyl groups) when the metal is Ca.  
 IT 24691-16-5F 24691-18-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 24691-16-5 HCAPLUS  
 CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate, (1R,5R)-rel- (CA INDEX NAME)

Relative stereochemistry.



RN 24691-18-7 HCAPLUS  
 CN Cyclohexanol, 3,3,5-trimethyl-, 1-acetate, (1R,5S)-rel- (CA INDEX NAME)

Relative stereochemistry.



L37 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN

AN 1968:29434 HCAPLUS Full-text

DN 68:29434

OREF 68:5687a,5690a

TI 3,5,5-Trimethylcyclohexanol esters

IN Buzas, Andre

PA Laboratoires Bruneau et Cie.

SO Fr., 2 pp.

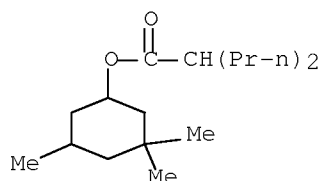
CODEN: FRXXAK

DT Patent

LA French

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 1476627		19670414	FR	19651220 <--
GI	For diagram(s), see printed CA Issue.				
AB	The preparation of esters of 3,5,5-trimethylcyclohexanol (I) which are of pharmacol. interest is described. I is treated either with the appropriate acid and a suitable catalyst, or with the corresponding acid chloride or anhydride in the presence of an amine e.g. pyridine. For example, I and m-(trifluoromethyl)phenyl- $\alpha$ -hydroxyacetic acid is refluxed in C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub> with 0.5% H <sub>2</sub> SO <sub>4</sub> for 7 hrs. The mixture is neutralized and the organic layer washed, dried, and distilled to give 85% 3,5,5-trimethylcyclohexyl m-(trifluoromethyl)phenyl- $\alpha$ -hydroxyacetate, m. 82°, b <sub>1</sub> 158°. Similarly prepared are the following II (R, % yield and phys. property given): m-F <sub>3</sub> CC <sub>6</sub> H <sub>4</sub> OCH <sub>2</sub> , 60, b <sub>20</sub> 193°; Pr <sub>2</sub> CH, 82, b <sub>25</sub> 165-7°; p-ClC <sub>6</sub> H <sub>4</sub> OCH <sub>2</sub> , 90, m. 92°.				
IT	17564-82-8F RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)				
RN	17564-82-8 HCAPLUS				
CN	Valeric acid, 2-propyl-, 3,3,5-trimethylcyclohexyl ester (8CI) (CA INDEX NAME)				



=> => d his

(FILE 'HOME' ENTERED AT 09:41:15 ON 27 OCT 2008)  
SET COST OFF

FILE 'HCAPLUS' ENTERED AT 09:41:30 ON 27 OCT 2008

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L2      329 S E3-E23/CO,PA,CS
      E E15+ALL
L3      1136 S E2+RT OR E2-E28/CS,PA
      E KUHN/AU
L4      11 S E3
      E KUHN W/AU
L5      550 S E3-E14,E16-E20
      E KUEHN/AU
L6      2 S E3
      E KUEHN W/AU
L7      192 S E3-E6,E8-E9
      E KEUHN/AU
      E SURBURG/AU
L8      79 S E4,E6
      E SUERBURG/AU
L9      1 S L1 AND L2-L8
      SEL RN

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FILE 'REGISTRY' ENTERED AT 09:44:04 ON 27 OCT 2008

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L13     1 S L12 CSS SAM
L14     432 S L12 CSS FUL
      SAV TEMP L14 GRESO565A/A
L15     274 S L14 NOT STEREO?/FS
L16     58 S L15 AND 1/NC AND 3/ELC.SUB
L17     23 S L16 AND 1/NR
L18     13 S L17 AND 2/O
L19     11 S L18 NOT PMS/CI
L20     158 S L14 NOT L15
L21     28 S L20 AND 1/NC AND 3/ELC.SUB AND 1/NR
L22     12 S L21 NOT L11
L23     5 S L22 AND 2/O
L24     3 S L23 NOT PMS/CI
L25     30 S L11,L19,L24
      SAV TEMP L25 GRESO565B/A

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FILE 'HCAPLUS' ENTERED AT 09:51:25 ON 27 OCT 2008

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L26     51 S L25
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L28     8 S L26 AND PY<=2004 NOT P/DT
L29     27 S L26 AND (PD<=20040630 OR PRD<=20040630 OR AD<=20040630) AND P
L30     35 S L28,L29
L31     3 S L30 AND L11
L32     4 S L27,L31
L33     1 S L30 AND L24
L34     5 S L32,L33
L35     30 S L30 NOT L34
      SEL AN 16 19 21
L36     3 S L35 AND E23-E28
L37     8 S L34,L36

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FILE 'REGISTRY' ENTERED AT 09:58:14 ON 27 OCT 2008

FILE 'HCAPLUS' ENTERED AT 09:58:28 ON 27 OCT 2008



SEL RN 3 L37

FILE 'REGISTRY' ENTERED AT 09:59:41 ON 27 OCT 2008

L38	42 S E29-E70
L39	37 S L38 NOT L25
L40	0 S L39 AND L14

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